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Research and Development Report

A FORTRAN IV CRYSTALLOGRAPHIC
SYSTEM OF PROGRAMS FOR
GENERALIZED SUPERPOSITIONS

by

Camden R. Hubbard and
Robert A. Jacobson

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November 1969

Ames Laboratory

at

Iowa State University of Science and Technology

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Camden R. Hubbard and Robert A. Jacobson

ABSTRACT

The system of three programs calculates symmetry and general superposition maps for triclinic, monoclinic, and orthorhombic space groups. The program GEN generates the basic direct access data set. The program SYMM calculates a direct access symmetry map. The program ALS calculates a superposition map using the minimum function with weighting, origin shift, and multiple superposition options. ALS uses direct access storage to keep computer storage at a minimum. A detailed description of the use of the programs together with symbolic program listings is supplied.

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I. Introduction

This report describes the use of three programs in use at the Ames Laboratory using the IBM 360/65. The programs are GEN, ALS, and SYMM. GEN writes a direct access Patterson data set from the sequential Patterson data set written by ALF (Ames Lab Patterson and Fourier program). The direct access data set is the basic data used by SYMM and ALS. SYMM writes a direct access symmetry map using the direct access Patterson data set. The Ames Laboratory superposition program, ALS - A General Superposition Program in Fortran IV, was written to satisfy four requirements: (1) small computer core allocation, (2) high speed execution, (3) generalized superpositions using the minimum function, and (4) weighting, origin shift, and multiple superposition options.

All three programs are written in FORTRAN IV to facilitate general use, changes, and improvements. Detailed instructions and program listings are included. The program listings contain example job control cards and DD cards for running each program at the Iowa State Computation Center. The parameters of the DD cards are appropriate for the example discussed in Part V.

As these programs are still being tested and improved, programming bugs not found in previous tests may still exist. Thus care should be exercised to ensure that the programs are working properly for each problem.

II. GEN - A Program to Create a Direct Access Patterson Data Set

A. General description

GEN is used to convert a Patterson map written as a sequential data set with one line of four-byte integer words per record into a direct access ¹ data set with one layer of two-byte integer words per record. The Patterson map must repeat the cell edges, i.e. $P(0,V,W)=P(XGRID,V,W)$ for all V and W. GEN is written in FORTRAN IV to facilitate changes and general use. The use of FORTRAN requires that the dimension and DEFINE FILE parameters must be integer constants. Thus, two dimension statements and the DEFINE FILE statement must be changed for each new problem. The data set name and space parameters on the necessary DD cards also must be changed. Symmetry restrictions are discussed in Section B, Part IV.

B. DIMENSION and DEFINE FILE parameters

Three statements within the program must be changed to fit each problem. These are the DEFINE FILE, DIMENSION, and INTEGER*2 statements. In general these statements should be typed

```
DIMENSION  LINE(NX)
INTEGER*2  LAYER(NX,NY)
DEFINE FILE 9(NL,NWORD,U,ID)
```

¹For a detailed discussion of the direct access Input-Output statements see "IBM System/360 FORTRAN IV Language," Form C28-6515-6, pp. 62-68.

The underlined parameters are user options defined as

NX = the number of grid points across the layer²

NY = the number of grid points down the layer

NL = the number of layers

NWORD = the number of four-byte words per layer (record)
 (=NX*NY/2 rounded up if necessary)

C. Control input data

Only one input card is needed. This card is described below.

<u>Column</u>	<u>Variable</u>	<u>Format</u>	<u>Value</u>
1-5	NX	I5	= the number of grid points across the layer of the Patterson
6-10	NY	I5	= the number of grid points down the layer of the Patterson
11-15	NL	I5	= the number of layers

(These variables are equivalent to those discussed in Section B)

D. DD cards

Two DD cards are required by GEN. Unit 10 is reserved for reading the sequential data set containing the output of the Patterson map from ALF or another Patterson program. Unit 9 is reserved for writing the permanent direct access layered data set. These two DD cards should be typed as follows:

²Counting for NX, NY, NL begins with 1. If the Patterson program numbers the grid points from 0 to XGRID across the layer, then NX=XGRID+1.

```
//GO.FT09FO01 DD DSN=dsname,UNIT=DISK,
// VOLUME=(PRIVATE,RETAIN,SER=XTALOG),SPACE=(NB,(NL,1),RLSE),
// DCB=BUFNO=1,DISP=(NEW,CATLG,DELETE)

// GO.FT10FO01 DD DSN=&&XXXX,DISP=(OLD,DELETE),
// UNIT=(DISK,,DEFER)
```

The underlined parameters are user options. NB = the number of bytes per record (layer) (thus $NB = 4 * NWORD$), NL = the number of layers, dsname represents a permissible data set name, and &&XXXX represents the temporary data set name used in ALF's //MAP DD card.

III. SYMM - Symmetry Map Program

A. General description

SYMM was written to create a direct access symmetry map using the Patterson data set written by GEN. The coordinate systems used in the program are: (1) X across the page, Y down the page, and Z for layers in the symmetry map and (2) U across the page, V down the page, and W for layers in the Patterson map. The symmetry map is generated in four steps. First, a point XYZ in electron density space is selected. Second, the N Harker vectors between the N symmetry related positions and XYZ are evaluated. Third, the maximum of the Patterson values $P(U,V,W)$, $P(U\pm 1,V,W)$, and $P(U,V,X\pm 1)$ is evaluated for the N Harker vectors.³

³For most symmetry operations the Harker peak will occur on a plane or a line. Thus a maximum of five or three Patterson values could be used. However, using the maximum of seven Patterson values simplifies the programming and will not significantly decrease the information in the symmetry map.

Fourth, the value of the symmetry map at XYZ is chosen as the minimum of these N values. Step three is performed to prevent loss of information and to broaden the resultant peaks. Since SYMM was written to handle an arbitrary number of symmetry operations (≥ 20), the unique region of the Patterson must be stored in core.

Two statements must be retyped for each problem. These statements are the DEFINE FILE and INTEGER*2 statements. Their parameters are discussed in Section B. The necessary region size (core allocation) for SYMM depends primarily on the volume of the Patterson map. The region size may be estimated by the approximation

$$32,000 + 2 * (NX) * (NY) * (NL + 2) + 10,000 \text{ bytes.}$$

The 32,000 represents the program size excluding the array allocation. The 10,000 bytes represents the system plus buffer allocations. The remaining term can be broken into two parts. The first, $NX * NY * (NL + 1) * 2$ is due to the array allocation necessary for the Patterson (symmetry unique region only) and a layer of the symmetry map. The second, $NX * NY * 2$ is for a buffer region for output of the direct access maps.

SYMM calculates a symmetry map of the same dimensions as the Patterson. If the Patterson is orthorhombic, then the symmetry map will have dimensions $NX = XGRID/2 + 1$, $NY = YGRID/2 + 1$, $NL = ZGRID/2 + 1$ (identical with the Patterson).

B. INTEGER*2 and DEFINE FILE parameters

Since SYMM is written in FORTRAN IV, the INTEGER*2 and DEFINE FILE parameters must be integer constants.

These two statements should be typed

```
DEFINE FILE 9(NL,NWORD,U,ID1), 10(NL,NWORD,U,ID2)
INTEGER* 2 MAP(NX,NY,NL), MAP2(NX,NY)
```

The underlined parameters are user options and are defined as

NX = the number of grid points across the layer
of the Patterson

NY = the number of grid points down the layer of the
Patterson

NL = the number of layers

NWORD = the number of storage words per record (layer)
and is $NX \times NY / 2$ rounded up if necessary.

(counting for NX, NY, NL begins with 1)

C. Control input data

Two types of input are required by SYMM - from magnetic disk and from punched cards. The Patterson map on disk created by GEN is referenced by DD cards (section D).

The data cards are described below.

Card No.	Column	Variable	Format	Value
1	1-80	TITLE	20A4	Alphanumeric title
2	1-5	NOV	I5	Number of Harker vector sets to be read
	6-10	IDENT	I5	Patterson symmetry code = 1 for 2/m = 2 for mmm

Card No.	Column	Variable	Format	Value
				Dimensions of Patterson map
	11-15	XYZMOD(1)	I5	= No. of grid points across layer
	16-20	XYZMOD(2)	I5	= No. of grid points down layer
	21-25	XYZMOD(3)	I5	= No. of layers (Counting begins with zero)
	26-30	XYZGRD(1)	I5	Full unit cell dimensions = No. of grid points across layer
	31-35	XYZGRD(2)	I5	= No. of grid points down layer
	36-40	XYZGRD(3)	I5	= No. of layers (Counting begins with zero)
	41-45	MAX	I5	Maximum peak height on Patterson
	46-50	CONS	I5	Constant added to each point in map
	51-55	NEG	I5	= T if all negative values in resultant map are set to 0 = F otherwise
3	1-80	FMT	20A4	Output format for one line of symmetry map enclosed in parentheses If XYZMOD(1) = 25 then (1H,2X,I2,2X,26I3,2X,I2) would be a possible format. The 1H is the carriage control. Both I2's are for line numbers; and the 26I3 is for the map.

4-5	1-80	LABH	33A4	Horizontal map label (two cards)
	1-52			LABH is intended for grid point indexing across the page.

6-5+NOV (T(K,I),(M(K,I,J),J=1,3), I=1,3) 12I5

The NOV Harker vector sets are input one vector per card. Each coordinate of a Harker vector K is represented by a translational component and three coordinate multipliers. For example,

$$\begin{aligned} U(K) &= T(K,1) + M(K,1,1)*X + M(K,1,2)*Y + M(K,1,3)*Z \\ V(K) &= T(K,2) + M(K,2,1)*X + M(K,2,2)*Y + M(K,2,3)*Z \\ W(K) &= T(K,3) + M(K,3,1)*X + M(K,3,2)*Y + M(K,3,3)*Z. \end{aligned}$$

The coordinate system used by SYMM is U and X across the layer, V and Y down the layer, and W and Z for layers.

Only the N Harker vectors between the atom at XYZ and the N symmetry related atoms are input to SYMM.

D. DD cards

DD cards are used to reference data sets on magnetic disk. Unit FT09 is reserved for reading the direct access Patterson written by GEN and unit FT10 is reserved for writing the symmetry map. These two sets of cards should be typed as follows

```
//GO.FT09FOO1 DD DSNAME=dsname1,DISP=(OLD,KEEP),UNIT=(DISK,,DEFER)
//GO.FT10FOO1 DD DSNAME=dsname2,DISP=(NEW,CATLG),UNIT=DISK,
// VOLUME=(PRIVATE,RETAIN,SER=XTALOG),SPACE=(NB,(NL,1),RLSE),
// DCB=BUFNO=1
```


Where

dsname1 = the data set name used in GEN for the Patterson
 dsname2 = a new data set name (must be unique)
 NB = 4*NWORD = the number of bytes per record
 (layer); and
 NL = the number of records (layers) to be written.

IV. ALS - A General Superposition Program in FORTRAN IV

A. General description and flow chart

ALS was written to satisfy the four requirements mentioned in the introduction. In ALS all superpositions, up to 10, are calculated for a given layer of the resultant map before proceeding to the next layer. This technique requires that only two 2-dimensional arrays be stored in the computer. The first array, M1, will be a layer of the Patterson map; the second array, M2, may be a layer of symmetry map, Patterson map, or previous superposition map. These arrays are updated by reading direct access data sets stored on magnetic disks.

Only the symmetry unique regions of the Patterson and symmetry map are stored on disk. Symmetry related regions are generated within ALS consistent with one of the three Patterson symmetry options: $\bar{1}$, 2/m, or mmm. The array M2, which has the dimensions of a layer of the full unit cell is filled using the specified symmetry option (Patterson-Patterson or Patterson-symmetry map superpositions only). The Patterson or symmetry map is also shifted on filling M2 according to the designated origin shift. If M2 is filled from a previous superposition result, no origin shift can be performed.

Multiple superpositions are easily handled. The user has two options: (1) to calculate all N superpositions in one run or (2) to calculate M ($<N$) superpositions, store the intermediate map on disk, and then calculate the remaining $N-M$ superpositions starting with the intermediate map. The second option is quite useful if investigation of the intermediate map is required before further superpositions can be calculated.

To facilitate high speed execution, input read delays are nearly eliminated by using two input units, one for each array, and the direct access statement `FIND(IQ'IZ)`. The statement `FIND(IQ'IZ)` buffers the layer IZ of the map stored on unit IQ into the buffer region of the computer. For example, if the statement `FIND(10'5)` is subsequently followed by `READ(10'5) MAP`, the fifth layer of the map stored on unit 10 is transferred from the buffer region to the array storage. If sufficient computation is done between the `FIND` and `READ` statements, no time is lost positioning the reading head of the disk unit or transferring data from the disk into the buffer region of the computer. In ALS the following calculations are performed for the layer between each `FIND` and `READ` statement: (1) application of the shift vector, (2) evaluation of linear interpolation between grid points within the layer, and (3) calculation of the minimum function.

Since ALS is written in FORTRAN IV, the DEFINE FILE and INTEGER*2 parameters must be changed to fit each problem. These changes are discussed in Section C. In Section B the restrictions which Patterson symmetry places upon array dimensions and orientation are discussed. The generation of the initial Patterson map is performed by GEN; however, if a Patterson-Patterson superposition is desired, a duplicate Patterson must be created. The copying of the original Patterson is discussed in Section E. Input control parameters are described in Section D. A general flow chart of ALS is shown in Table I, page 12.

B. Map Symmetry⁴

Triclinic Patterson Map

The general Patterson function is

$$P(UVW) = \frac{1}{V} \sum_{hkl}^{\infty} |F_{hkl}|^2 \cos 2\pi(hU+kV+lW).$$

Thus the Patterson map is centric, and one half of the Patterson volume is unique. The inversion center is the only Patterson symmetry for a triclinic system. In ALS any layer with $W > 1/2$ can be generated from the region of the Patterson with $W < 1/2$ since $P(UVW) = P(1-U, 1-V, 1-W)$. For a triclinic system the unique region of the Patterson must be stored on disk. For ALS the unique region is defined

⁴Tetragonal, cubic, hexagonal, or trigonal Patterson symmetry cannot be handled explicitly by ALS. However if a sufficient fraction of the unit cell of the Patterson is calculated, the remainder can be generated using one of the symmetry options: $\bar{1}$, $2/m$, mmm .

TABLE I

as full in U (0 to XGRID along x)⁵
 full in V (0 to YGRID along y)
 half in W (0 to ZGRID/2 along z).

The number ZGRID will be even since the W = 1/2 layer must be input.

Monoclinic Pattern Map

The Patterson function for a b-unique Patterson is

$$P(UVW) = \frac{4}{V} \sum_{hkl}^{\infty} (|F_{hkl}|^2 \cos 2\pi(hU+lW) + |F_{\bar{h}kl}|^2 \cos 2\pi(hU-lW)) \cos 2\pi kV$$

The two symmetry relations which follow from this equation are $P(UVW) = P(U, 1-V, W)$ and $P(UVW) = P(1-U, V, 1-W)$. These symmetry operations correspond to a mirror perpendicular to V at $V=1/2$ and to a two-fold axis along the line $1/2, V, 1/2$. ALS uses these relations by requiring that the monoclinic Patterson be layered perpendicular to the unique axis.

The unique region of the Patterson which is stored is

half in U (0 to XGRID/2 along x)
 half in V (0 to ZGRID/2 along z, the unique and layer axis)
 full in W (0 to YGRID along y).

⁵x,y,z represent the coordinate system of the program. z is the layer direction, x across the layer, and y down the layer. Numbering of grid points and layers begins with zero as this is normal convention.

The monoclinic map must be stored with layers containing U and W. The numbers XGRID and YGRID must both be even.

Orthorhombic Patterson Map

The Patterson function for an orthorhombic Patterson is

$$P(UVW) = \frac{8}{V} \sum_0^{\infty} |F_{hkl}|^2 \cos 2\pi hU \cos 2\pi kV \cos 2\pi lW.$$

The unique region of the Patterson which must be stored is

half in U (0 to XGRID/2 along x)
 half in V (0 to YGRID/2 along y)
 half in W (0 to ZGRID/2 along z).

The values XGRID, YGRID, and ZGRID must be even.

Symmetry Maps

Since a symmetry map is formed from Harker layers, lines, or points of the Patterson, the symmetry of the symmetry map is generally higher than the symmetry of the Patterson. ALS requires that the symmetry map is input either on unit FT12 with the dimensions of the full unit cell, or input on unit FT13 as a map with dimensions identical with those of the Patterson and symmetry related regions generated using the same symmetry operation as indicated for the Patterson.

C. INTEGER*2 and DEFINE FILE parameters

Array Dimensions

Dimensions for arrays M1 and M2 are user options and must be changed to fit each problem. Both arrays are declared INTEGER*2 to save memory storage. The INTEGER*2 statement should be typed

```
INTEGER*2 M1(a,b), M2(c,d)
```

where a,b,c, and d are integer constants. The array M2 is dimensioned for a layer of the full unit cell ($c=XGRID+1$, $d=YGRID+1$). The array M1 is dimensioned for a layer of the unique region of the Patterson map. For example, if the Patterson has 2/m symmetry then $a=1+XGRID/2$ and $b=1+YGRID$.

DEFINE FILE parameters

The general form of the FORTRAN define file statement is

```
DEFINE FILE a1(m1,r1,f1,v1),a2(m2,r2,f2,v2), ....
```

ALS requires four different input-output files. These are units $a_1=11$, $a_2=12$, $a_3=13$, and $a_4=10$. The f_i indicate the input-output mode and are equal to U for all four units. The v_i are called the associated variables which point to the record that immediately follows the last record transmitted. In ALS the v_i are $v_1=ID1$, $v_2=ID2$, $v_3=ID3$, and $v_4=ID4$. The values m_i and r_i specify the number of records and the size of each record, respectively.

Specifically,

$m_1=m_3$ = number of layers in the Patterson (=ZGRID/2 + 1)

$m_2=m_4$ = number of layers in the full unit cell

(= $2*m_1-1=ZGRID+1$)

$r_1=r_3$ = $a*b/2$ rounded up if necessary

$r_2=r_4$ = $c*d/2$ rounded up if necessary

(a,b,c,d are as defined in INTEGER*2 parameters above).

D. Control input data

Two types of input are required by ALS. These are direct access data sets on magnetic disks and data cards. The program GEN creates the data set on disk and this data set is referenced by DD cards (section E). The necessary data cards are discussed below.

Card No.	Column	Variable	Format	Value
1	1-80	TITLE	20A4	Alphanumeric title
2	1-5	IM2	I5	= 1 if full map is to be input on unit FT12 = 2 if Patterson or symmetry map input on FT13
	6-10	IOUT	I5	= 0 resultant map printed only = 1 resultant map printed and written on FT10 = 2 resultant map output on FT10 only
	11-15	ICLASS	I5	= 1 for triclinic Patterson = 2 for monoclinic Patterson = 3 for orthorhombic Patterson

Card No.	Column	Variable	Format	Value
	16-20	NSUP	I5	Number of superpositions ≤ 10
	21-25	XGRID	I5	Number of grid points across full unit cell (Counting begins with zero)
	26-30	YGRID	I5	Number of grid points down full unit cell (Counting begins with zero)
	31-35	ZGRID	I5	Number of layers in full unit cell (Counting begins with zero)
	36-40	CONS	I5	Constant to be added to Patterson and/or symmetry map before weighting
	41-45	NEG	L5	= T if all negative values are to be set to zero = F otherwise
	46-50	SCALE	F5.2	Multiplicative scaling factor for resulting map
<hr/>				
3	1-5	XSTART	I5	Starting grid point across the layer for resulting map (≥ 0)
	6-10	XEND	I5	Final Grid point across the layer ($\leq$ XGRID)
	11-15	YSTART	I5	Starting grid point down the layer (≥ 0)
	16-20	YEND	I5	Final grid point down the layer ($\leq$ YGRID)

Card No.	Column	Variable	Format	Value
	21-25	ZSTART	I5	Initial layer (≥ 0)
	26-30	ZEND	I5	Final layer
	31-35	XO	I5	X origin
	36-40	YO	I5	Y origin
	41-45	ZO	I5	Z origin

The origin location XO,YO,ZO will be shifted to the origin (0,0,0) of the resultant map. The START and END values correspond to the shifted map.

*** omit this card if IOU=2 ***

4	1-80	FMT	20A4	Output format for a line of the resultant map. Each line will consist of a line number, line of map, and a line number. The format should have a carriage control and be enclosed in parentheses. If XSTART=0 and XEND=25, then the format could be (1H_,2X,I2,2X,26I3,2X,I2).
---	------	-----	------	---

*** omit these two cards if IOU=2 ***

5 and 6	1-80 1-52	LABH	33A4	Horizontal map label. LABH is output above and below each layer to provide grid point indexing.
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7 to NSUP+6

	1-10	FXS	F10.2	X-shift vector
	11-20	FYS	F10.2	Y-shift vector
	21-30	ZS	I10	Z-shift vector
	31-40	WS	F10.2	Weighting factor for shifted map

(FXS,FYS,ZS) is the shift vector for shifting the origin of the Patterson with respect to the origin of the symmetry map, duplicate Patterson, or previous superposition result. Linear interpolation between grid points if calculated within each layer but not between layers.

E. DD cards

DD cards are required to reference a data set on magnetic disk. DD cards should be inserted between the /* and the //GO.SYSIN DD * statements only if the data set will be required by ALS. Possible DD cards needed by ALS are listed below with their use.

** to reference the original Patterson data set created by GEN **
 //GO.FT11FOO1 DD DSNAME=dsname1,DISP=(OLD,KEEP),
 // UNIT=(DISK,,DEFER),DCB=BUFNO=1

** to reference a full map created during a previous superposition **
 //GO.FT12FOO1 DD DSNAME=dsname2,DISP=(OLD,KEEP),
 // UNIT=(DISK,,DEFER),DCB=BUFNO=1

** to reference a duplicate Patterson created by IEBGENER **
 //GO.FT13FOO1 DD DSNAME=&&YYYY,DISP=(OLD,DELETE),
 // UNIT=(DISK,,DEFER),DCB=BUFNO=1

** to reference a symmetry map created by SYMM **
 //GO.FT13FOO1 DD DSNAME=dsname3,DISP=(OLD,KEEP)
 // UNIT=(DISK,,DEFER),DCB=BUFNO=1

** to create a new data set containing the resultant full superposition map on disk **
 //GO.FT10FOO1 DD DSNAME=dsname4,DISP=(NEW,CATLG),
 // UNIT=DISK,SPACE=(NB,(NL,1)),
 // VOLUME=(PRIVATE,RETAIN,SER=XTALOG),DCB=BUFNO=1

where

dsnamei is a unique data set name,
 &&YYYY is a label for a temporary data set,
 NB is the number of bytes per record (layer), and
 NL is the number of records (layers) to be written.

F. Duplicating a Patterson data set

If a Patterson-Patterson superposition is to be calculated, two identical maps must exist on two different magnetic disks. The system utility program IEBGENER can be used to copy the direct access data set onto a scratch disk. IEBGENER reads and rewrites the Patterson data set as if it were a sequential data set. The necessary control and DD cards are listed below.

```
//PASS EXEC PGM=IEBGENER
//SYSPRINT DD SYSOUT=A
//SYSUT1 DD DSN=dsname,DISP=(OLD,KEEP),UNIT=(DISK,,DEFER),
//  VOLUME=(PRIVATE,RETAIN,SER=XTALOG),DCB=(RECFM=F,BLKSIZE=NB)
//SYSUT2 DD DSN=&&YYYY,DISP=(NEW,PASS),SPACE=(NB,(NL,1)),
//  UNIT=DISK,DCB=(RECFM=F,BLKSIZE=NB)
//SYSIN DD DUMMY
/*
```

where

dsname is the data set name for the Patterson map,
 &&YYYY is a temporary data set label,
 NB is the number of bytes per record(layer), and
 NL is the number of records.

G. Estimating core allocation

Necessary core allocation for ALS at the Iowa State Computation Center can be approximated by the following formula (in bytes):

$$\text{REGION SIZE} \approx 33,000 + 2*(a*b + c*d) + \text{RDB} + 12,000.$$

The value 33,000 represents the size of the program excluding the INTEGER*2 arrays M1 and M2. The value 12,000 approximates the region necessary for the IBM system. The expression $2*(a*b + c*d)$ is the number of bytes of core necessary for arrays M1 and M2. RDB (region for disk buffers) depends on the size of the arrays, IM2 (map input mode), and IOUT (superposition map output mode). Buffer allocation is needed only for units actually used by ALS. The possibilities contributing to RDB are

<u>Unit</u>	<u>Usage</u>	<u>Buffer size</u>	
FT11	always	$2*a*b$	
FT13	IM2=2	$2*a*b$	each value should be rounded up to nearest 2048 before adding
FT12	IM2=1	$2*c*d$	
FT10	IOUT=2 or 3	$2*c*d$	

(The values a,b,c,d are defined in Section C, INTEGER*2 parameters.)

V. Example and Program Listing

The program listings for GEN, ALS, and SYMM contain the job control cards necessary for the IBM 360/65 operating system at the Iowa State Computation Center. The parameters in the DEFINE FILE and dimension statements and the DD cards correspond to the example discussed below. The CPU (central processing unit) time and necessary "GO" step region size are given below.

A. Example

Crystal Dataspace group: $P2_1/c$ lattice constants: $a=10.93$, $b=7.07$, $c=12.07$, $\beta=117.63^\circ$ Map Symmetry and Orientation

Since the unit cell is monoclinic, the Patterson must have each layer bounded by a and c (layer axis is b). The unique region is 0 to $1/2$ along a , 0 to 1 along c , and 0 to $1/2$ along b . The number of grid points were chosen as 46 along a , 50 along c , and 28 along b for the full unit cell.

ALF⁶

The control parameter IWANT was preceded by a 1 to store the computed sharpened Patterson on disk. The necessary DD card was

```
//MAP DD DSNAME=dsname,DISP=(NEW,CATLG),UNIT=DISK,
// SPACE=(804,(100,15),RLSE),VOLUME=(PRIVATE,RETAIN,SER=XTALOG),
// DCB=(RECFM=VB,LRECL=100,BLKSIZE=804)
```

GEN

CPU time = 1.6 sec

Region size = 64K

SYMM

A symmetry map with the same dimensions as the Patterson was calculated using the three Harker vectors

⁶ALF: A General Fourier Program in PL1 for Triclinic, Monoclinic, and Orthorhombic Space Groups, J. Rodgers and R. A. Jacobson, Iowa State University, IS-2155, 1969.

$$(UVW)_1 = (-2X, -2Y, -2Z), (UVW)_2 = (2X, 1/2 - 2Y, -1/2),$$

$$(UVW)_3 = (0, 1/2, 1/2 - 2Z).$$

CPU time = 116.8

Region size = 96K

ALS

Four superpositions of the Patterson on the symmetry map were calculated for one-half the unit cell (full x full x half).

CPU time = 53.4 sec

Region size = 64K

PROGRAM LISTINGS

GEN

```
//BOXXGEN JOB 'XXXXX,TIME=1,REGION=96K',USER,CLASS=D
//GEN EXEC FORTG,TIME.GO=1
//FORT.SYSIN DD *
C   GEN CONVERTS THE LINE DATA SET WRITTEN BY A PATTERSON PROGRAM      GEN 001
C   INTO A LAYERED DIRECT ACCESS DATA SET WITH INTEGER*2 WORDS(2 BYTE) GEN 002
C                                                                           GEN 003
C   THE DEFINE FILE AND DIMENSIONS MUST BE CHANGED TO FIT EACH PROBLEM GEN 004
C   DIMENSION LINE(NX)                                                  GEN 005
C   INTEGER*2 LAYER(NX,NY)                                              GEN 006
C   DEFINE FILE 9(NL,NWORD,U,ID)                                       GEN 007
C       WHERE NX =NUMBER OF GRID POINTS PER LINE ACROSS THE PAGE      GEN 008
C       AND NY EQUALS THE NUMBER OF LINES PER LAYER.  BOTH NUMBERS    GEN 009
C       ARE = GRID+1 OR GRID/2+1                                       GEN 010
C       WHERE NL=NUMBER OF LAYERS AND NWORDS = THE NUMBER OF STORAGE   GEN 011
C       WORDS PER LAYER =(NX*NY)/2 ROUNDED UP IF NECESSARY            GEN 012
C       DEFINE FILE 9(15,612,U,ID)                                     GEN 013
C       INTEGER*2 LAYER(24,51)                                         GEN 014
C       DIMENSION LINE(24)                                             GEN 015
C   READ IN CONTROL CARD                                               GEN 016
C   READ(1,1) NX,NY,NL                                                GEN 017
C   1 FORMAT(3I5)                                                       GEN 018
C   WRITE(3,2) NX,NY,NL                                                GEN 019
C   2 FORMAT(1H1,T10,'***CONTROL INFORMATION***'/1H ,T10,I3,'= NUMBER OF GEN 020
C   1 POINTS PER LINE'/1H ,T10,I3,'= NUMBER OF LINES PER LAYER'/1H , GEN 021
C   2 T10,I3,'= NUMBER OF LAYERS')                                     GEN 022
C   LAY=1                                                                GEN 023
C   9 LINES=1                                                            GEN 024
C   10 READ(10) LINE                                                    GEN 025
C       DO 12 I=1,NX                                                    GEN 026
C   12 LAYER(I,LINES)=LINE(I)                                           GEN 027
C       LINES=LINES+1                                                    GEN 028
C       IF(LINES.LE.NY) GOTO 10                                         GEN 029
C       WRITE(9,LAY) LAYER                                              GEN 030
C       WRITE(3,20) LAY                                                 GEN 031
C   20 FORMAT(1H0,T10,'RECORD NO.',I3,' WRITTEN ON FT09')             GEN 032
C       LAY=LAY+1                                                        GEN 033
C       IF(LAY.LE.NL) GOTO 9                                             GEN 034
C       STOP                                                            GEN 035
C       END                                                            GEN 036
/*
//GO.FT10F001 DD DSN=SEQ.XXXXXLIN,DISP=(OLD,KEEP),UNIT=(DISK,,DEFER)
//GO.FT09F001 DD DSN=SEQ.XXXXXPAT,DISP=(NEW,CATLG,DELETE),UNIT=DISK,
// VOLUME=(PRIVATE,RETAIN,SER=XTALOG),SPACE=(2448,(15,1)),DCB=BUFNO=1
//GO.SYSIN DD *
24 51 15
/*
```


SYMM

```

//ROXXSYM JOB 'XXXXX,TIME=3,SIZE=96K,LINES=4',USER,CLASS=D
//S1 EXEC FORTG,LINES=4,TIME.GO=3,REGION.GO=96K
//FORT.SYSIN DD *
C *** SYMM *** A GENERAL SYMMETRY MAP PROGRAM
C ----- SYMM 001
C CARD VARIABLE FORMAT COMMENT SYMM 002
C ----- SYMM 003
C 1 TITLE 20A4 ALPHANUMERIC TITLE SYMM 004
C ----- SYMM 005
C 2 NOV I5 NO. OF HARKER VECTOR SETS SYMM 007
C IDENT I5 =1 IF 2/M PATTERSON SYMMETRY SYMM 008
C =2 IF MMM PATTERSON SYMMETRY SYMM 009
C XYZMOD(I),I=1,3 3I5 = NO. OF PATTERSON GRID POINTS SYMM 010
C ACROSS PAGE, DOWN PAGE, AND IN SYMM 011
C LAYERS. NUMBERING BEGINS WITH SYMM 012
C ZERO AND ENDS WITH XYZMOD(I) SYMM 013
C XYZGRD(I),I=1,3 3I5 = NO. OF FULL CELL GRID POINTS SYMM 014
C ACROSS PAGE, DOWN PAGE, AND IN SYMM 015
C LAYERS. NUMBERING BEGINS WITH SYMM 016
C ZERO AND ENDS WITH XYZMOD(I) SYMM 017
C MAX I5 =MAXIMUM PEAK HEIGHT ON PATTERSONSYMM 018
C CONS I5 = CONSTANT TO BE ADDED TO MAP SYMM 019
C NEG L5 =T IF ALL NEGATIVE VALUES SET=0 SYMM 020
C =F OTHERWISE SYMM 021
C ----- SYMM 022
C 3 FMT 20A4 OUTPUT FORMAT FOR PRINTED MAP SYMM 023
C ----- SYMM 024
C 4 LABH(I),I=1,33 33A4 HORIZONTAL MAP LABEL (2 CARDS) SYMM 025
C ----- SYMM 026
C 5 - 4+NOV (T(K,I),(M(K,I,J), J=1,3), I=1,3) 12I5 SYMM 027
C ..... EXPLANATION..... SYMM 028
C THE NOV HARKER VECTOR SETS ARE INPUT ONE VECTOR PER CARD. EACH SYMM 029
C COORDINATE OF A HARKER VECTOR K IS REPRESENTED BY A TRANSLATIONAL SYMM 030
C COMPONENT AND THREE COORDINATE MULTIPLIERS. FOR EXAMPLE SYMM 031
C SYMM 032
C  $U(K) = T(K,1) + M(K,1,1)*X + M(K,1,2)*Y + M(K,1,3)*Z$  SYMM 033
C  $V(K) = T(K,2) + M(K,2,1)*X + M(K,2,2)*Y + M(K,2,3)*Z$  SYMM 034
C  $W(K) = T(K,3) + M(K,3,1)*X + M(K,3,2)*Y + M(K,3,3)*Z$  SYMM 035
C SYMM 036
C THE COORDINATE SYSTEM USED BY SYMM IS SYMM 037
C U AND X ACROSS THE PAGE, SYMM 038
C V AND Y DOWN THE PAGE, AND SYMM 039
C W AND Z FOR LAYERS. SYMM 040
C SYMM 041
C FOR THE HARKER VECTOR (1/2-2X,1/2+2Y,1/2-2Z) WITH 74,30,52 GRID SYMM 042
C POINTS ALONG U,V,W RESP. THEN THE ONLY NON ZERO T'S AND M'S ARE SYMM 043
C  $T(K,1)=37$ ,  $M(K,1,1)=-2$ ;  $T(K,2)=15$ ,  $M(K,2,2)=+2$ ;  $T(K,3)=26$ , AND SYMM 044
C  $M(K,3,3)=-2$ . SYMM 045
C FOR THE TRIGONAL HARKER VECTOR (X+Y,X+2Y,0) THE ONLY NON ZERO SYMM 046
C T'S AND M'S ARE  $M(K,1,1)=1$ ,  $M(K,1,2)=1$ ;  $M(K,2,1)=1$ ,  $M(K,2,2)=2$ . SYMM 047
C ----- SYMM 048
C SYMM 049
C THE DEFINE FILE AND INTEGER*2 STATEMENTS MUST BE CHANGED FOR EACH SYMM 050
C PROBLEM SYMM 051
C DEFINE FILE 9(15,612,U, ID1), 10(15,612,U, ID2) SYMM 052
C INTEGER*2 MAP(24,51,15) MAP2(24,51) SYMM 053
C SYMM 054
C COMMON XYZMOD,XYZGRD,IDENT,CONS,IVX,IVY,IVZ,IP SYMM 055
C INTEGER*2 XYZMOD(3),XYZGRD(3), T(20,3), M(20,3,3), LABV(200) SYMM 056
C DIMENSION FMT(20), TITLE(20), LABH(33),TYPE(5,2) SYMM 057
C INTEGER X,Y,Z,A,B,C,CONS SYMM 058

```

```

LOGICAL NEG
DATA TYPE/'MONOCLINIC PATTERSONORTHORHOMBIC PAT.  '/'
READ(1,1010) TITLE
WRITE(3,1100) TITLE
READ(1,1000) NOV,IDENT,XYZMOD,XYZGRD,MAX,CONS,NEG
WRITE(3,1030)
WRITE(3,1040) XYZGRD
WRITE(3,1045)
WRITE(3,1040) XYZMOD
WRITE(3,1050) NOV
READ(1,1010) FMT
READ(1,1010) LABH
READ(1,1020)((T(A,B), (M(A,B,C),C=1,3),B=1,3), A=1,NOV)
REWIND 1
WRITE(3,1060)(A,(T(A,B), (M(A,B,C),C=1,3),B=1,3), A=1,NOV)
WRITE(3,1070) (TYPE(I,IDENT),I=1,5),MAX,CONS,NEG
NXRA = XYZMOD(1) + 1
NYRA = XYZMOD(2) + 1
NZRA = XYZMOD(3) + 1
DO 10 LAY=1,NZRA
10 READ(9'LAY) ((MAP(I,J,LAY),I=1,NXRA),J=1,NYRA)
REWIND 9
DO 35 I=1,200
35 LABV(I)=I-1
DO 80 LAY=1,NZRA
DO 75 IX=1,NXRA
DO 75 IY=1,NYRA
X=IX-1
Y=IY-1
Z=LAY-1
IPEAK=MAX
DO 50 A=1,NOV
IVX= T(A,1)+ M(A,1,1)*X+M(A,1,2)*Y+ M(A,1,3)*Z
IVY= T(A,2)+ M(A,2,1)*X+M(A,2,2)*Y+ M(A,2,3)*Z
IVZ= T(A,3)+ M(A,3,1)*X+M(A,3,2)*Y+ M(A,3,3)*Z
CALL SEVEN(MAP,NXRA,NYRA,NZRA)
IPEAK= MINO(IP,IPEAK)
50 CONTINUE
IF( NEG .AND. IPFAK.LT.0) IPEAK=0
MAP2(IX,IY)=IPEAK
75 CONTINUE
WRITE(10'LAY) MAP2
WRITE(3,1100) TITLE
WRITE(3,1080) Z,XYZGRD(3)
WRITE(3,1090) LABH
WRITE(3,FMT) ((LABV(J),(MAP2(I,J),I=1,NXRA),LABV(J)),J=1,NYRA)
WRITE(3,1090) LABH
80 CONTINUE
C
C.....FORMAT STATEMENTS.....
C
1000 FORMAT(10I5,L5)
1010 FORMAT(20A4)
1020 FORMAT(12I5)
1030 FORMAT(1H0,T5,'*** FULL PATTERSON DIMENSIONS ***')
1040 FORMAT(1H0,T10,'GRID POINTS ACROSS THE PAGE FROM 0 TO ',I3/
' 1H ,T10,'GRID POINTS DOWN THE PAGE FROM 0 TO ',I3/
2 1H ,T10,'AND LAYERS FROM 0 TO ',I3)
1045 FORMAT(1H0,T5,'*** DIMENSIONS FOR UNIQUE REGION OF PATTERSON ***')
1050 FORMAT(1H0,T5,'***',I3,' INPUT VECTOR SETS ***'/1H ,T10,'COORDINATES
1E SYSTEM IS'/1H ,T15,'X ACROSS THE PAGE'/1H ,T15,'Y DOWN THE PAGE')

```

```

      2 / 1H ,T15,'Z FOR LAYERS')
1060 FORMAT(1H0,T10,'VECTOR SET NO. ',I3/ 1H ,T10,'U=',T15,I3,'+',I3, SYMM 120
      1 ' *X +', I3, ' *Y +', I3, ' *Z' ,/1H ,T10,'V=',T15,I3,'+',I3, SYMM 121
      2 ' *X +', I3, ' *Y +', I3, ' *Z' ,/1H ,T10,'W=',T15,I3,'+',I3, SYMM 122
      3 ' *X +', I3, ' *Y +', I3, ' *Z' ) SYMM 123
1070 FORMAT(1H0,T10,5A4/1H ,T10,'MAX PEAK HEIGHT =' ,I8/1H ,T10, SYMM 124
      1 'CONSTANT ADDED TO MAP=' ,I3/1H ,T10,'NEGATIVE POINTS SET =0',L3) SYMM 125
1080 FORMAT(1H0,T10,'***** LAYER',I3,' OF',I3,' *****') SYMM 126
1090 FORMAT(1H0,33A4/) SYMM 127
1100 FORMAT(1H1,20X,20A4) SYMM 128
      STOP SYMM 129
      END SYMM 130
      SUBROUTINE SEVEN(MAP,XS,YS,ZS) SYMM 131
      INTEGER X,Y,Z,CONS,XS,YS,ZS SYMM 132
      COMMON XYZMOD,XYZGRD,IDENT,CONS,X,Y,Z,IPEAK SYMM 133
      INTEGER*2 MAP(XS,YS,ZS),XYZMOD(3),XYZGRD(3) ,XYZ(3) SYMM 134
      DIMENSION M7(7) SYMM 135
      J=0 SYMM 136
      XYZ(1)=X SYMM 137
      XYZ(2)=Y SYMM 138
      XYZ(3)=Z SYMM 139
      1 J=J+1 SYMM 140
      IF(IDENT.EQ.1) GO TO 4 SYMM 141
      DO 2 I=1,3 SYMM 142
      DO 2 K=1,2 SYMM 143
      IF(XYZ(I).LT.0) XYZ(I)=XYZ(I)+XYZGRD(I) SYMM 144
      IF(XYZ(I).GT.XYZGRD(I)) XYZ(I)=XYZ(I)-XYZGRD(I) SYMM 145
      2 IF(XYZ(I).GT.XYZMOD(I)) XYZ(I)=XYZGRD(I)-XYZ(I) SYMM 146
      GO TO 6 SYMM 147
      4 DO 5 I=1,3 SYMM 148
      DO 5 K=1,2 SYMM 149
      IF(XYZ(I).GT.XYZGRD(I)) XYZ(I)=XYZ(I)-XYZGRD(I) SYMM 150
      5 IF(XYZ(I).LT.0) XYZ(I) = XYZ(I) + XYZGRD(I) SYMM 151
      IF(XYZ(3).GT.XYZMOD(3)) XYZ(3)=XYZGRD(3)-XYZ(3) SYMM 152
      IF(XYZ(1).LE.XYZMOD(1)) GO TO 6 SYMM 153
      XYZ(1) = XYZGRD(1) - XYZ(1) SYMM 154
      XYZ(2)=XYZGRD(2)-XYZ(2) SYMM 155
      6 L=XYZ(1)+1 SYMM 156
      M=XYZ(2)+1 SYMM 157
      N=XYZ(3)+1 SYMM 158
      M7(J)=MAP(L,M,N) SYMM 159
      GO TO (10,20,30,40,50,60,70),J SYMM 160
      10 XYZ(1)=X-1 SYMM 161
      GO TO 1 SYMM 162
      20 XYZ(1)=X+1 SYMM 163
      GO TO 1 SYMM 164
      30 XYZ(1)=X SYMM 165
      XYZ(2)=Y-1 SYMM 166
      GO TO 1 SYMM 167
      40 XYZ(2)=Y+1 SYMM 168
      GO TO 1 SYMM 169
      50 XYZ(2)=Y SYMM 170
      XYZ(3)=Z-1 SYMM 171
      GO TO 1 SYMM 172
      60 XYZ(3)=Z+1 SYMM 173
      GO TO 1 SYMM 174
      70 IPEAK=MAX0(M7(1),M7(2),M7(3),M7(4),M7(5),M7(6),M7(7))+CONS SYMM 175
      RETURN SYMM 176
      END SYMM 177
/*
//GO,FT09F001 DD DSNAME=SEQ.XXXXXPAT,UNIT=(DISK,,DEFER),DISP=(OLD,KEEP)

```

```
//GO.FT10F001 DD DSN=SEQ.XXXXXSYM,UNIT=DISK,DISP=(NEW,CATLG),
// SPACE=(2448,(15,1)),VOLUME=(PRIVATE,RETAIN,SER=XTALOG),DCB=BUFNO=1
//GO.SYSIN DD *
```

0.5

PI-CYCLOPENTADIENYL MANGANESE TRICARBONYL SYMM MAP

3 1 23 50 14 46 50 28 1000 0 F
(1H, I2, 3X, 24I3, 3X, I2)

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
---	---	---	---	---	---	---	---	---	---	----	----	----	----	----	----	----	----	----	----	----	----	----	----

-2 -2 -2

-2 25 -2 -14

25 14 -2

/ *

29
ALS

```
//BOXXSUP JOB 'XXXXX,TIME=4,LINES=3,REGION=96K',USER,CLASS=D
//ALS EXEC FORTG,TIME.GO=4,LINES=3,REGION.GO=64K
//FORT.SYSIN DD *
C*** ALS - AMES LAB FORTRAN SUPERPOSITION PROGRAM BY CAM HUBBARD ***
C
C-----
C CARD VARIABLE FORMAT COMMENT
C-----
C 1 TITLE (20A4) ALPHANUMERIC TITLE
C-----
C 2 IM2 (I5) =1 IF WHOLE MAP2 READ FROM FT12
C =2 IF MAP2 FORMED FROM FT13,
C USING THE SYMMETRY OF THE
C PATTERSON .
C IOUT (I5) =0 OUTPUT MAP PRINTED ONLY
C =1 RESULTANT MAP PRINTED AND
C WRITTEN ON FT10
C =2 OUTPUT ON FT10 ONLY
C ICLASS (I5) =1 TRICLINIC, =2 MONOCLINIC,
C =3 ORTHORHOMBIC (3 MIRRORS)
C NSUP (I5) NUMBER OF SUPERPOSITION (.LE. 10)
C XGRID (I5) GRID POINTS ACROSS FULL PAT
C YGRID (I5) GRID POINTS DOWN FULL PAT
C ZGRID (I5) NUMBER OF LAYERS IN FULL PAT
C CONS (I5) CONSTANT TO BE ADDED TO PATTERSON
C OR SYMMETRY MAP BEFORE WEIGHTING
C NEG (L5) =T IF ALL NEG VALUES ARE SET =0
C SCALE (F5.2) SCALING FACTOR FOR FINAL MAP
C-----
C 3 XSTART (I5) FIRST GRID POINT ACROSS PAGE
C XEND (I5) LAST GRID POINT ACROSS PAGE
C YSTART (I5) FIRST GRID POINT DOWN PAGE
C YEND (I5) LAST GRID POINT DOWN PAGE
C ZSTART (I5) INITIAL OUPUT SECTION IN Z
C ZEND (I5) FINAL OUTPUT SECTION IN Z
C XO (I5) X ORIGIN (INTEGER)
C YO (I5) Y ORIGIN (INTEGER)
C ZO (I5) Z ORIGIN (INTEGER)
C THE ORIGIN LOCATION (X0,Y0,Z0) WILL BE SHIFTED TO (0,0,0)
C-----
C *** OMIT THIS CARD IF OUT=2 ***
C 4 FMT (20A4) OUTPUT FORMAT
C-----
C *** OMIT THESE TWO CARDS IF IOUT=2 ***
C 5 LABH(I) (33A4) HORIZONTAL MAP LABEL, TWO CARDS
C-----
C 6 FXS (F10.2) X SHIFT VECTOR (DECIMAL)
C FYS (F10.2) Y SHIFT VECTOR (DECIMAL)
C ZS (I10) Z SHIFT VECTOR (INTEGER)
C W (F10.2) WEIGHTING FACTOR
C-----
C IMPLICIT INTEGER (X,Y,Z)
C
C THE FOLLOWING 3 CARDS DEPEND UPON THE SPECIFIC PROBLEM AND
C NEED TO BE CHANGE ONCE FOR EACH INVESTIGATION.
C
```

```

      INTEGER*2 M1(24,51), M2(47,51)
      DEFINE FILE 11(15,612,U,ID1), 12(29,1199,U,ID2), 13(15,612,U,ID3),
1 10(29,1199,U,ID4)
C
C
      LOGICAL NEG,IS,BAR1,BAR2
      INTEGER CONS
      DIMENSION TITLE(20),FMT(20),FXS(10),FYS(10),W(10),CLASS(6,3),
1 LABH(33),LABV(150), ZS(10)
      DATA CLASS/' TRICLINIC PATTERSON MONOCLINIC PATTERSON ORTHO
1 RHOMBIC PATTERSON '/
      READ(1,1008) TITLE
      READ(1,1003) IM2,IOUT,ICLASS,NSUP,XGRID,YGRID,ZGRID,CONS,NEG,SCALE
      READ(1,1004) XSTART,XEND,YSTART,YEND,ZSTART,ZEND,XO,YO,ZO
      WRITE(3,1001) TITLE
      WRITE(3,1002) (CLASS(I,ICLASS), I=1,6)
      WRITE(3,1005) NSUP,CONS,NEG,SCALE,IM2,IOUT
      WRITE(3,1006) XGRID,YGRID,ZGRID
      WRITE(3,1013) XO,YO,ZO
      WRITE(3,1007) XSTART,XEND,YSTART,YEND,ZSTART,ZEND
      IF(IOUT.LE.1) READ(1,1008) FMT,LABH
      READ(1,1009) (FXS(I), FYS(I), ZS(I), W(I), I=1,NSUP)
      WRITE(3,1011)
      WRITE(3,1012) (FXS(I), FYS(I), ZS(I), W(I), I=1,NSUP)
      DO 1 I=1,NSUP
      FXS(I)=FXS(I)-XO
      FYS(I)=FYS(I)-YO
      ZS(I)=ZS(I)-ZO
      IF(FXS(I).LT.0.0) FXS(I)=FXS(I)+XGRID
      IF(FYS(I).LT.0.0) FYS(I)=FYS(I)+YGRID
1 IF(ZS(I).LT.0) ZS(I)=ZS(I)+ZGRID
C
C SET UP BASIC CONTROL DATA
      ZLIM=ZGRID
      XSTART=XSTART+1
      YSTART=YSTART+1
      ZSTART=ZSTART+1
      XEND=XEND+1
      YEND=YEND+1
      ZEND=ZEND+1
      XGRID=XGRID+1
      YGRID=YGRID+1
      ZGRID=ZGRID+1
      ZMOD=ZGRID/2+1
      GOTO (2,3,4),ICLASS
2 XMOD=XGRID
  YMOD=YGRID
  GOTO 5
3 XMOD=XGRID/2+1
  YMOD=YGRID
  GOTO 5
4 XMOD=XGRID/2+1
  YMOD=YGRID/2+1
5 DO 6 J=YSTART,YEND
6 LABV(J)=J-1
C
C BEGIN SUPERPOSITIONS BY LAYERS IN Z
      DO 100 ZZ2=ZSTART,ZEND
      Z2=ZZ2+ZO
      IF(Z2.LE.0) Z2=ZGRID+Z2-1
      IF( Z2 .GT. ZGRID ) Z2= Z2-ZGRID+1

```

	IF(IM2.EQ.2) GOTO 8	ALS 120
C		ALS 121
C	MAP2 TO BE READ FROM FT12 (FULL ELECTRON DENSITY SPACE MAP)	ALS 122
C		ALS 123
	READ(12'Z2,ERR=9991) M2	ALS 124
	IF(ID2.LT.ZGRID) FIND(12'ID2)	ALS 125
	8 BAR1=.FALSE.	ALS 126
	IF(Z2.LE.ZMOD) GOTO 7	ALS 127
	Z2=ZGRID-Z2+1	ALS 128
	BAR1=.TRUE.	ALS 129
	7 ISUP=0	ALS 130
	IF(IM2.EQ.1) GOTO 22	ALS 131
C		ALS 132
C	M2 TO BE FORMED FROM M1 READ FROM FT13 WITH SAME SYMMETRY AS PAT	ALS 133
C		ALS 134
	10 READ(13'Z2,ERR=9991) M1	ALS 135
	IF(ID3.GT.ZMOD) ID3=ZGRID+1-ID3	ALS 136
	FIND(13'ID3)	ALS 137
	GOTO (11,15,17), ICLASS	ALS 138
C		ALS 139
C	TRICLINIC PATTERSON (CENTER AT 1/2,1/2,1/2)	ALS 140
C		ALS 141
	11 DO 14 I=1,XGRID	ALS 142
	DO 14 J=1,YGRID	ALS 143
	II=I-X0	ALS 144
	JJ=J-Y0	ALS 145
	IF(.NOT. BAR1) GOTO 12	ALS 146
	II=XGRID-I+1-X0	ALS 147
	JJ=YGRID-J+1-Y0	ALS 148
	12 IF(II.LE.0) II=II+XGRID-1	ALS 149
	IF(JJ.LE.0) JJ=JJ+YGRID-1	ALS 150
	14 M2(II,JJ)=M1(I,J)	ALS 151
	GOTO 19	ALS 152
C		ALS 153
C	MONOCLINIC PATTERSON (MIRROR AT Z=1/2, CENTER AT 1/2,1/2,Z)	ALS 154
C		ALS 155
	15 DO 16 I=1,XMOD	ALS 156
	DO 16 J=1,YGRID	ALS 157
	II=I-X0	ALS 158
	JJ=J-Y0	ALS 159
	IF(II.LE.0) II=II+XGRID-1	ALS 160
	IF(JJ.LE.0) JJ=JJ+YGRID-1	ALS 161
	M2(II,JJ)=M1(I,J)	ALS 162
	II=XGRID-I+1-X0	ALS 163
	JJ=YGRID-J+1-Y0	ALS 164
	IF(II.LE.0) II=II+XGRID-1	ALS 165
	IF(JJ.LE.0) JJ=JJ+YGRID-1	ALS 166
	16 M2(II,JJ)=M1(I,J)	ALS 167
	GOTO 19	ALS 168
C		ALS 169
C	ORTHORHOMBIC PATTERSON (3MIRRORS)	ALS 170
C		ALS 171
	17 DO 18 II=1,XGRID	ALS 172
	DO 18 JJ=1,YGRID	ALS 173
	I=II+X0	ALS 174
	J=JJ+Y0	ALS 175
	IF(I.LE.0) I=I+XGRID-1	ALS 176
	IF(J.LE.0) J=J+YGRID-1	ALS 177
	IF(I.GT.XGRID) I=I-XGRID+1	ALS 178
	IF(J.GT.YGRID) J=J-YGRID+1	ALS 179
	IF(I.GT.XMOD) I=XGRID+1-I	ALS 180

IF(J.GT.YMOD) J=YGRID+1-J	ALS 181
18 M2(II,JJ)=M1(I,J)	ALS 182
C TAKE CARE OF UNIT CELL TRANSLATIONS	ALS 183
C	ALS 184
19 DO 20 I=1,XGRID	ALS 185
20 M2(I,YGRID)=M2(I,1)	ALS 186
DO 21 I=1,YGRID	ALS 187
21 M2(XGRID,I)=M2(1,I)	ALS 188
M2(XGRID,YGRID)=M2(1,1)	ALS 189
C	ALS 190
C MAP1 (PATTERSON) TO BE READ FROM FT11	ALS 191
C	ALS 192
22 ISUP= ISUP+1	ALS 193
Z1= ZZ2-ZS(ISUP)	ALS 194
23 IF(Z1.GT.0) GOTO 24	ALS 195
Z1=ZGRID+Z1-1	ALS 196
GOTO 23	ALS 197
24 IF(Z1.GT.ZGRID) Z1=Z1-ZGRID+1	ALS 198
BAR2=.FALSE.	ALS 199
IF(Z1.LE.ZMOD) GOTO 25	ALS 200
BAR2=.TRUE.	ALS 201
Z1=ZGRID+1-Z1	ALS 202
25 READ(11,Z1,ERR=9990) M1	ALS 203
IF(ISUP.EQ. NSUP) GOTO 26	ALS 204
ID1=ZZ2-ZS(ISUP+1)	ALS 205
GOTO 27	ALS 206
26 ID1=ZZ2+1-ZS(1)	ALS 207
27 IF(ID1.LE.0) ID1=ZGRID+ID1-1	ALS 208
IF(ID1.GT.ZGRID) ID1=ID1-ZGRID+1	ALS 209
IF(ID1.GT.ZMOD) ID1=ZGRID+1-ID1	ALS 210
FIND(11,ID1)	ALS 211
C	ALS 212
C DO SUPERPOSITION FOR ONE LAYER IN Z	ALS 213
C	ALS 214
30 XSHIFT=INT(FXS(ISUP))	ALS 215
YSHIFT=INT(FYS(ISUP))	ALS 216
FX0 = FXS(ISUP)-FLOAT(XSHIFT)	ALS 217
FY0 = FYS(ISUP)-FLOAT(YSHIFT)	ALS 218
34 FX1= 1.0 -FX0	ALS 219
FY1= 1.0 -FY0	ALS 220
DO 50 Y3=YSTART,YEND	ALS 221
Y1=Y3-YSHIFT	ALS 222
IF(ICLASS.EQ.1 .AND. BAR2) Y1=YSHIFT-Y3+2	ALS 223
IF(Y1 .LE. 0) Y1 = YGRID+Y1-1	ALS 224
IF(Y1.GT.YGRID) Y1=Y1-YGRID+1	ALS 225
YSAVE=Y1	ALS 226
DO 45 X3= XSTART,XEND	ALS 227
X1= X3-XSHIFT	ALS 228
IF(ICLASS.EQ.1 .AND. BAR2) X1=XSHIFT-X3+2	ALS 229
IF(X1 .LE. 0) X1 = XGRID+X1 -1	ALS 230
IF(X1.GT.XGRID) X1=X1-XGRID+1	ALS 231
Y1=YSAVE	ALS 232
GOTO (35,36,38),ICLASS	ALS 233
35 ISIGN=-1	ALS 234
IF(BAR2) ISIGN=1	ALS 235
X1P=X1+ISIGN	ALS 236
Y1P=Y1+ISIGN	ALS 237
IF(X1P.LE.0) X1P=XGRID+X1P-1	ALS 238
IF(Y1P.LE.0) Y1P=YGRID+Y1P-1	ALS 239
IF(X1P.GT.XGRID) X1P=X1P-XGRID+1	ALS 240
IF(Y1P.GT.YGRID) Y1P=Y1P-YGRID+1	ALS 241

	GOTO 41	ALS 242
36	ISIGN=-1	ALS 243
	IF(X1.LE.XMOD) GOTO 37	ALS 244
	X1=XGRID-X1+1	ALS 245
	Y1=YGRID-Y1+1	ALS 246
	ISIGN=+1	ALS 247
37	X1P=X1+ISIGN	ALS 248
	Y1P=Y1+ISIGN	ALS 249
	IF(X1P.LE.0) X1P=XGRID+X1P-1	ALS 250
	IF(Y1P.LE.0) Y1P=YGRID+Y1P-1	ALS 251
	IF(Y1P.GT.YGRID) Y1P=Y1P-YGRID+1	ALS 252
	IF(X1P.LE.XMOD) GOTO 41	ALS 253
	X1P=XGRID-X1P+1	ALS 254
	Y1P=YGRID-Y1P+1	ALS 255
	GOTO 41	ALS 256
38	ISIGNX=-1	ALS 257
	ISIGNY=-1	ALS 258
	IF(X1.LE.XMOD) GOTO 39	ALS 259
	ISIGNX=+1	ALS 260
	X1=XGRID-X1+1	ALS 261
39	IF(Y1.LE.YMOD) GOTO 40	ALS 262
	ISIGNY=+1	ALS 263
	Y1=YGRID-Y1+1	ALS 264
40	X1P=X1+ISIGNX	ALS 265
	Y1P=Y1+ISIGNY	ALS 266
	IF(X1P.LE.0) X1P=XGRID+X1P-1	ALS 267
	IF(Y1P.LE.0) Y1P=YGRID+Y1P-1	ALS 268
	IF(X1P.GT.XMOD) X1P=XGRID-X1P+1	ALS 269
	IF(Y1P.GT.YMOD) Y1P=YGRID-Y1P+1	ALS 270
C		ALS 271
C	DO X-Y INTERPOLATION	ALS 272
C		ALS 273
41	A1= FX1*M1(X1,Y1)+FX0*M1(X1P,Y1)	ALS 274
	A0= FX1*M1(X1,Y1P)+FX0*M1(X1P,Y1P)	ALS 275
	MAP1= W(ISUP)*(FY1*A1 +FY0*A0 +CONS)	ALS 276
	MAP2= M2(X3,Y3)	ALS 277
	IF(ISUP.EQ.1) MAP2=MAP2+CONS	ALS 278
	IF(NEG .AND. MAP1.LT.0) MAP1=0	ALS 279
	IF(NEG .AND. MAP2.LT.0) MAP2=0	ALS 280
	M2(X3,Y3)= MIN0(MAP1,MAP2) *SCALE	ALS 281
45	CONTINUE	ALS 282
50	CONTINUE	ALS 283
	IF(ISUP.LT.NSUP) GOTO 22	ALS 284
C		ALS 285
C	OUTPUT OF PARTICULAR LAYER OF FINAL MAP	ALS 286
C		ALS 287
	M2ZM1=ZZ2-1	ALS 288
	IF(IOUT .EQ.2) GOTO 85	ALS 289
	WRITE(3,1014) TITLE,M2ZM1,ZLIM	ALS 290
	WRITE(3,1015) LABH	ALS 291
	WRITE(3,FMT)(LABV(K),(M2(I,K),I=XSTART,XEND),LABV(K),	ALS 292
	1 K=YSTART,YEND)	ALS 293
	WRITE(3,1015)LABH	ALS 294
	IF(IOUT .EQ.0) GOTO 100	ALS 295
85	WRITE(10,ZZ2) M2	ALS 296
	WRITE(3,1016) ZZ2	ALS 297
100	CONTINUE	ALS 298
	GOTO 9999	ALS 299
9990	WRITE(3,1017)	ALS 300
	GOTO 9999	ALS 301
9991	WRITE(3,1018)	ALS 302

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C
C  FORMAT STATEMENTS
C
1001 FORMAT(1H1,T10,20A4)
1002 FORMAT(1H0,T10,6A4/)
1003 FORMAT( 8I5,L5,F5.3)
1004 FORMAT(9I5)
1005 FORMAT(/1H_,T10,'NUMBER OF SUPERPOSITIONS  =',I4 /
1      1H0,T10,'CONSTANT ADDED TO MAPS =',I7/1H ,T10,
2      'NEGATIVE POINTS SET=0 ',L9/1H ,T10,'SCALING FACTOR FOR MAP3 ',
3      F7.2,/1H ,T10, 'MAP2 INPUT MODE=', T39,I2/1H ,T10, 'MAP OUTPUT MO
4DE= ',T39,I2)
1006 FORMAT(1H0,T10,'FULL PATTERSON HAS THE FOLLOWING DIMENSIONS'/
1      1H ,T15,'GRID POINTS ACROSS THE PAGE =',I4/ 1H ,T15,'GRID POINTS
2DOWN  THE PAGE =',I4/ 1H ,T15,'AND THE NUMBER OF LAYERS  =',I4)
1007 FORMAT(1H0,T10,'THE SUPERPOSITION MAP WILL HAVE THE FOLLOWING DIME
1NSIONS'/ 1H ,T15, 'GRID POINTS ACROSS THE PAGE FROM',I4,' TO',I4/
2      1H ,T15, 'GRID POINTS DOWN  THE PAGE FROM',I4,' TO',I4/
3      1H ,T15, 'AND LAYERS  FROM',I4,' TO',I4)
1008 FORMAT(20A4)
1009 FORMAT(2F10.2,I10,1F10.2)
1011 FORMAT( 1H0, T10,'SHIFT VECTOR', T36,'WEIGHT'/1H ,T10,
1      '0' X Y Z)')
1012 FORMAT(1H ,T11,2F5.1,I5,11X,F5.2)
1013 FORMAT( 1H0,T10, 'ORIGIN SHIFT',T25, 'X0=',I3/ 1H ,T25, 'Y0=',I3/
1      1H ,T25,'Z0=',I3)
1014 FORMAT(1H1,T15,20A4/1H , 'LAYER',I3,' OF',I3)
1015 FORMAT(1H0,33A4/)
1016 FORMAT(1H ,T10,'RECORD NO. =',I3,' WRITTEN ON FT10')
1017 FORMAT(1H ,T10,'ERR IN READING FT11')
1018 FORMAT(1H ,T10,'ERR IN READING FT12')
9999 STOP
      END
/*
//GO.FT10F001 DD DSNAME=SEQ.XXXXXSUP,DISP=(NEW,CATLG),UNIT=DISK,
// VOLUME=(PRIVATE,RETAIN,SER=XTALOG),SPACE=(4794,(29,1)),DCB=BUFNO=1
//GO.FT11F001 DD DSNAME=SEQ.XXXXXPAT,UNIT=(DISK,,DEFER),
// DISP=(OLD,KEEP),DCB=BUFNO=1
//GO.FT13F001 DD DSNAME=SEQ.XXXXXSYM,DISP=(OLD,DELETE),
// UNIT=(DISK,,DEFER),DCB=BUFNO=1
//GO.SYSIN DD *
PI-CYCLOPENTADIENYL MANGANESE TRICARBONYL PATTERSON-SYMM MAP SUPERPOSITION
      2      2      2      4      46      50      28      0      T      1.0
      0      46      0      50      0      14      0      0      0
12.0          14.5          0      1.0
-12.0         -14.5          0      1.0
-12.0          10.5         -14      1.0
12.0          39.5          14      1.0
/*

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ALS 303
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